VCU Innovation Gateway
Office of the Vice President for Research and Innovation

Carbon Allotrope

A Recipe for the Design of Penta-graphene

Metastable structures of matter can provide an array of favorable electronic and mechanical properties relative to their ground state. However, many of these potential metastable structures are not experimentally explored due to their high energy barriers and therefore low realizability. Current theoretical approaches of identifying metastable structures only explore potential energy surfaces of structures with high realizabilities. Researchers at Virginia Commonwealth University have developed a roadmap to enhance the realizabilities of previously dismissed structures and allow for the synthesis of desired metastable 2D carbon allotropes.

The technology

This roadmap utilizes topologically assembled precursors (TAP) that are prevented from accessing the ground state or other isomers through three steps: (1) A precursor molecule that resembles the atomic, structural, and local symmetry of the desired structure is selected that (2) is then made into different topological assemblies. This is achieved by confining the precursor units into constrained superlattices and controlling their overall orientation to induce connectivity between certain atomic nodes of adjacent units. (3) These topological assemblies are then relaxed using density functional theory to their nearest potential energy surface critical point. The use of this roadmap has been suggested for the synthesis of penta-graphene, composed only of carbon pentagons, via the precursor molecule 3,3-dimethyl-1-butene (C_6H_{12}). Theoretical calculation suggest that this carbon polymorph is dynamically and mechanically stable, temperature resistant up to 1000 K, has an ultrahigh ideal strength that outperforms graphene, and an intrinsic quasi-direct band gap as large as 3.25 eV.

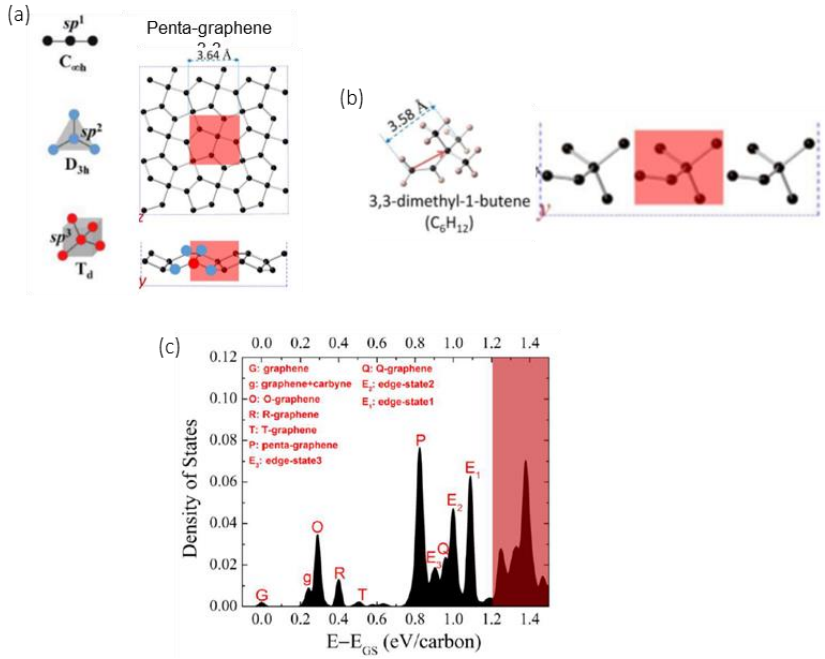

Figure 1. (a) sp1, sp2 and sp3 carbons and views of penta-graphene down the z and y axes. (b) Precursor molecule 3,3-dimethyl-1-butene and a lateral view (y) when aligned. (c) The relative probability of different structures vs. their energy above the ground state. Penta-graphene has a high realizablity while the realizability of graphene is suppressed based on peak height.

Benefits

- Guide for synthesizing novel metastable structures
- Favorable optical, mechanical, and electrical properties of penta-graphene

Applications

- Energy
  - More efficient and lighter batteries
  - High Li^+ coordinating ability
  - Renewable energy power storage
- Electronics
  - Miniaturization of technology
  - Semiconductors
  - Touch screens
- Composite/coating reinforcement
- Biomedical
  - Biosensors
  - Antimicrobial surfaces
  - Drug delivery
  - Tissue engineering

Patent status:
Patent pending: US20190228842A1

License status:
This technology is available for licensing to industry for further development and commercialization.

Category:
Engineering and Physical Science

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External resources:
Zhang, et. al. (2015)

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